Nanodroplets on Metal Surfaces: Wetting, Spreading and Interface Formation

Edmund B. Webb III, Gary S. Grest, and David R. Heine

Sandia National Laboratories; Albuquerque, NM

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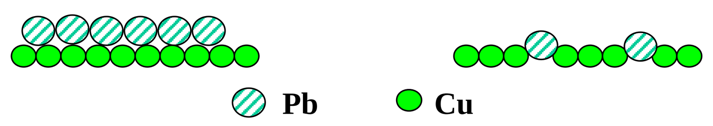
Motivation

- **Develop a more fundamental understanding of fluid transport on metal surfaces**
  - **joining metals (brazing, soldering)**
  - **growth of metal interfaces (thin films, self assembly)**
- **Pb on Cu(111) and Cu(100) displays rich phase behavior**
  - **Pb on Cu is partially wetting (θ_{eq} ~ 50° - 20°) [1,2]**
  - **coverage dependent surface phases form on Cu (111) and (100) [2,3]**
  - **D_{Pb} high for overlayer phases … low for surface alloy phases [2]**



- **experimentally observed 'foot' diffuses out from islands/drops with $R \sim t^{1/2}$ [2,3]**

[1] – Bailey and Watkins; Proc. Phys. Soc. 63(1949)350
[2] – J. Moon, *et al*; Surface Science 488(2001)73-82
[3] – G. Prévot, *et al*; Phys Rev B 61(2000)10393

Model – Embedded Atom Method

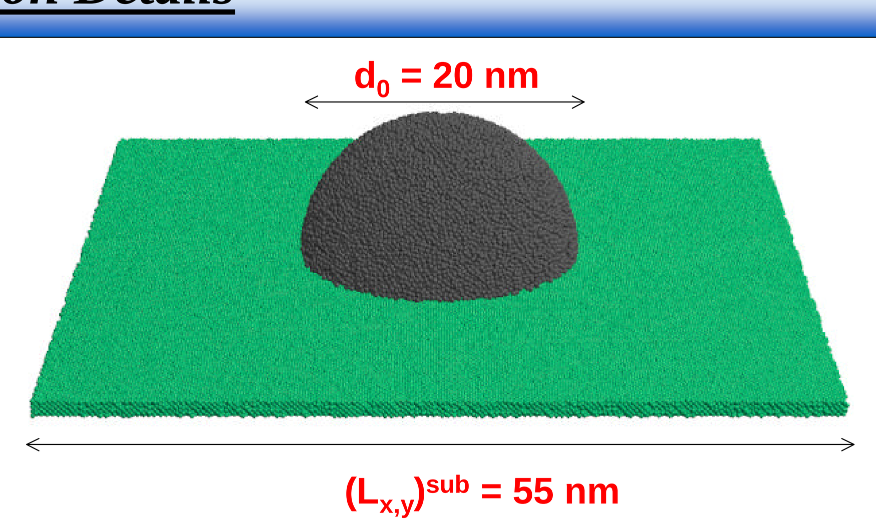
$$E_i = F_i(\rho_i) + \tfrac{1}{2}\sum_{j\neq i}\Phi_{ij}(R_{ij})$$

$$\rho_i = \sum_{j\neq i}\rho_j^a(R_{ij})$$

- **Multi-body potential (captures the nature of bonding in metals)**
- **Pb and Cu potentials from literature [1,2]; Pb/Cu cross-term recently published [3]**
  - **$(T_m)^{Pb}$ = 600 K {experiment}; $(T_m)^{Pb}$ = 618 K {model}**
  - **$(T_m)^{Cu}$ = 1353 K {experiment}; $(T_m)^{Cu}$ = 1278 K {model}**
- **New potential accurately predicts binary properties (phase diagram, heat of mixing)**

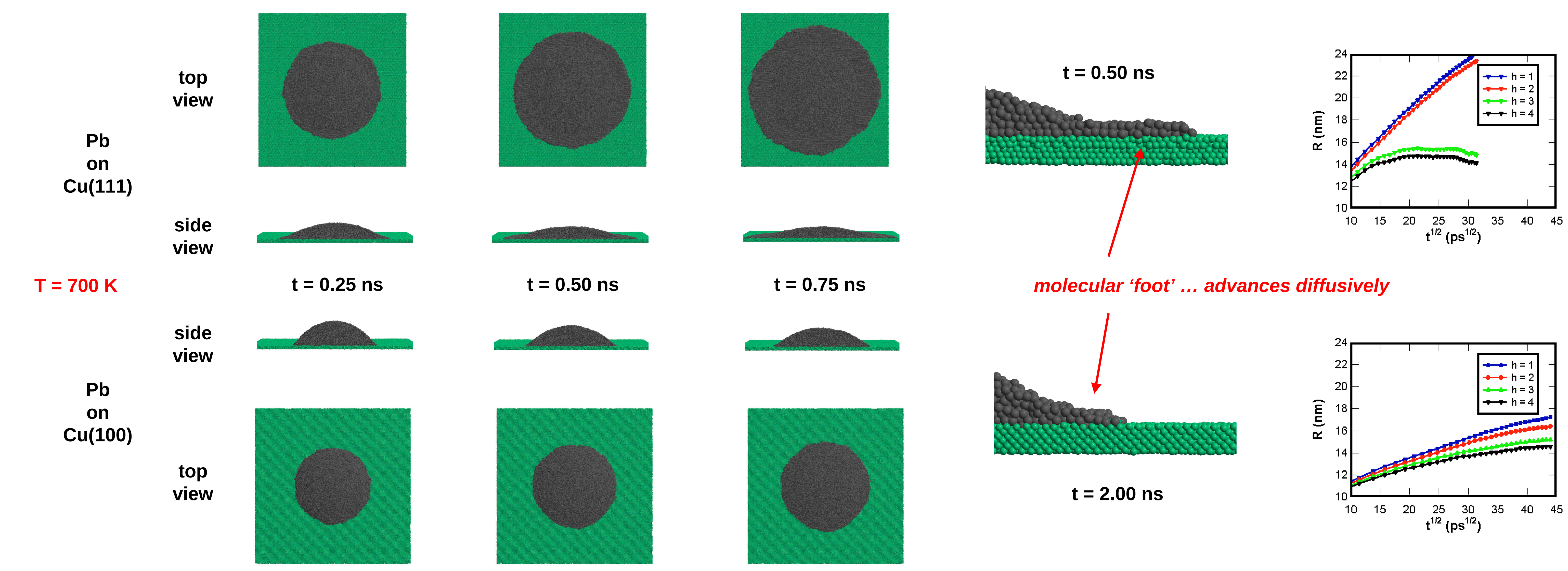
[1] – H.S. Lim, *et al*; Surf. Sci. 269/270(1992)1109
[2] – S.M. Foiles, *et al*; Phys. Rev. B 33(1986)7983
[3] – J.J. Hoyt; *et al*; Modelling Simul. Mater. Sci. Eng. 11(2003)1

Simulation Details

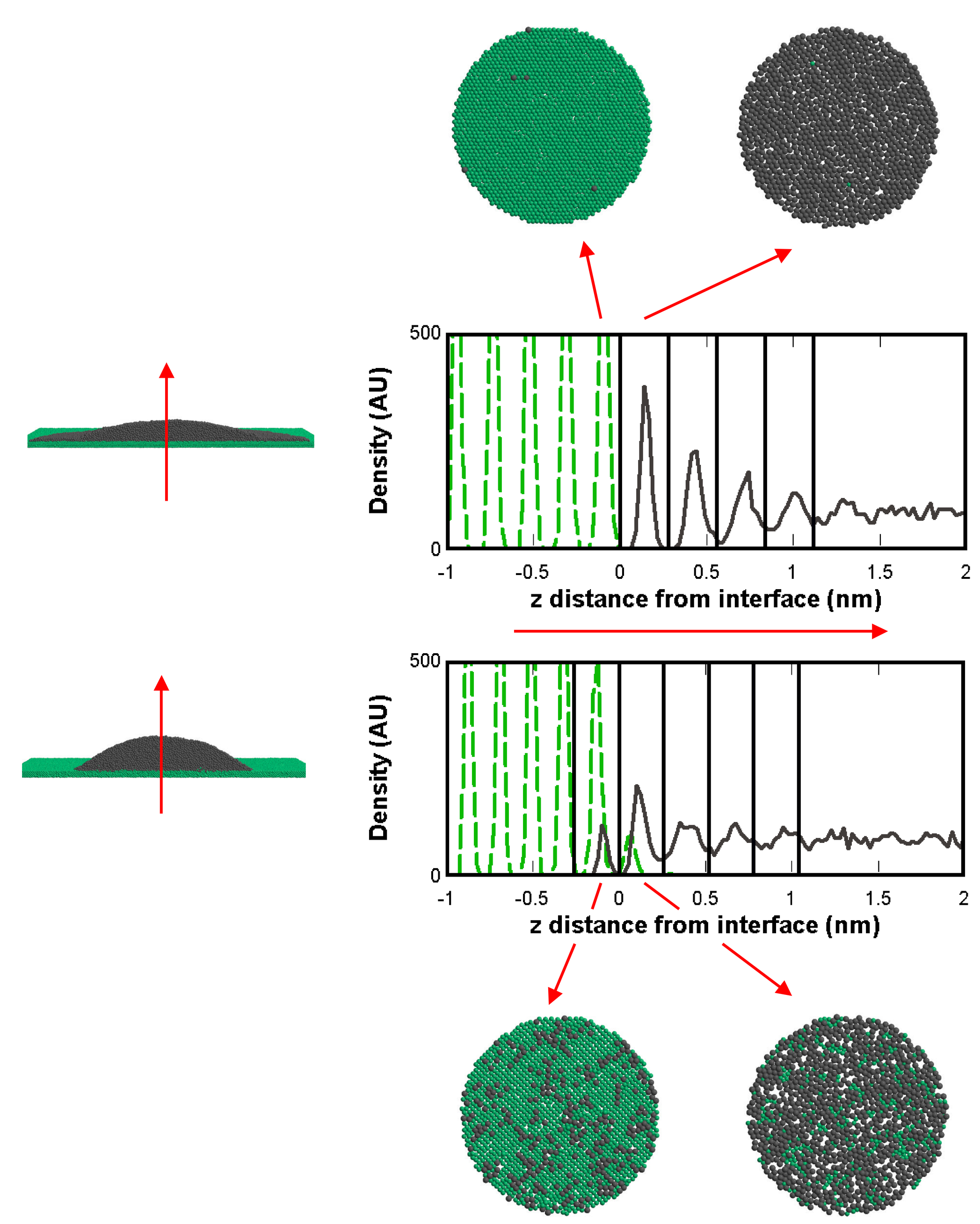


- **NVT ensemble (periodic boundary conditions in x and y … z is ⊥ to interface)**
- **$(T_m)^{Pb}$ < {T_{sim} = 700 K} < $(T_m)^{Cu}$**

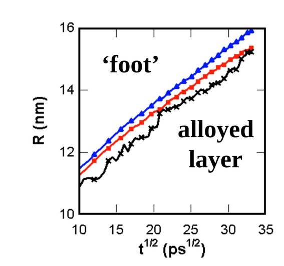
Simulation Results – Dynamics of Spreading



Simulation Results – Interfacial Structure

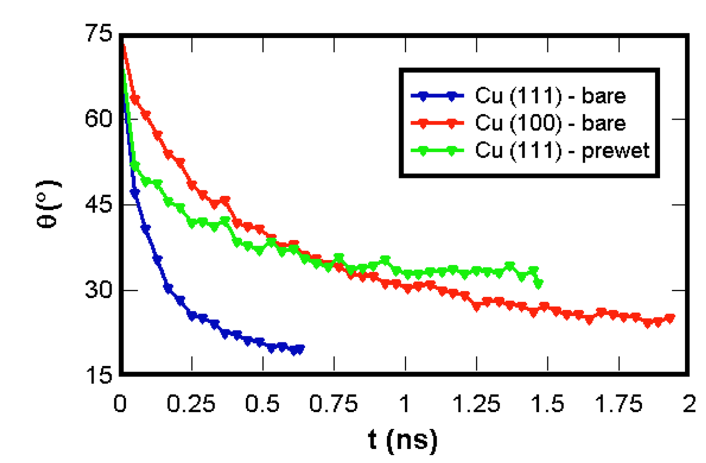


- **A surface alloying reaction that occurs on Cu(100), but is absent on Cu(111), directly controls spreading rate**
- **Data for radial growth of alloyed layer directly follows 'foot' data on Cu(100)**



Conclusions / Future

- **On both Cu surfaces, kinetics of drop spreading are controlled by 'foot' kinetics**



- **Simulations on *prewet* surfaces show equilibrium contact angle ~30º**
- **Action of 'foot' decreases effective friction on Cu(111) and increases it on Cu(100)**

- **Complete simulations of wetting on prewet Cu(100)**
- **Determine specific mechanisms by which 'foot' advances on each substrate**

- **Excellent qualitative agreement with experiment (slow on Cu(100) where alloyed structure exists; fast on Cu(111) where overlayer structure exists)**
- ***Can experiment confirm/refute structure of film observed in simulations?***